STRUCTURAL STUDY OF A KAOLINITE SINGLE-CRYSTAL USING PED AND DIFFRACTION TOMOGRAPHY

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Kaolinite is an abundant submicrometer-sized "TO"-type dioctahedral sheet silicate [$Al_2Si_2O_5(OH)_4$]. Its building units are the infinite 2D layers of corners shared SiO_4 tetrahedra and edge connected $Al_2O_2(OH)_4$ octahedra. Except of ZVYAGIN's (1960) oblique texture patterns based structure solution, X-ray and neutron diffraction methods were used on powdered samples.

The structure of a kaolinite *single crystal* from Mád (Hungary) was solved using precession electron diffraction (VINCENT & MIDGLEY, 1994; OWN, 2005; AVILOV *et al.*, 2007) and the newly developed technique of electron-diffraction tomography (KOLB *et al.*, 2007, 2008). The data collection was carried out using a Tecnai G^2X transmission electron microscope equipped with a CeB_6 gun operating at 200 kV and a tomography holder with a tilt range up to ±70°. We acquired intensities from 90° large wedge of reciprocal space within 0.8 Å resolution limit using a 4 Mb, 16 bits, Eagle CCD detector.

Structure of kaolinite was determined in the SIR2008 (implemented in the Il Milione package; BURLA *et al.*, 2007) and refined to R1 = 0.227, wR^2 = 0.547 using 236 observed unique reflections in SHELX97 (SHELDRICK, 2008). As a result we described kaolinite in the *C*1 triclinic space group (a = 5.056 Å, b = 9.122 Å, c = 7.250 Å, α = 88.72°, β = 104.18°, γ = 90.25°). Largest deviations are within a ± 0.36 value in the differential Fourier-map.

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Atom coordinates and isotropic displacement parameters for kaolinite of Mád, Hungary.

Atom	x	y	z	U_{iso}
Si1	0.429	0.930	0.425	0.024
Si2	0.919	0.764	0.449	0.024
Al2	0.714	1.106	0.836	0.027
Al3	0.716	0.770	0.834	0.008
O1	0.544	0.933	0.691	0.001
O2	0.458	1.125	0.953	0.017
O3	0.464	1.222	0.666	0.017
O4	0.620	0.832	0.380	0.013
O5	0.438	1.088	0.393	0.019
O6	0.967	1.256	0.934	0.003
O7	0.899	0.944	0.893	0.068
O8	0.141	0.857	0.369	0.035
O9	1.026	1.118	0.713	0.016